Collaboration Ignites Laser Advances

View of a target shot in the Omega target chamber. The 60-beam Omega laser system is a 40-kilojoule, direct-drive laser located at the Laboratory for Laser Energetics (LLE) at the University of Rochester. Collaborations between LLE and Livermore's Laser Programs have been of mutual benefit to both organizations.

RAMPANT, occasionally rancorous, competition among scientists, institutions, and schools of thought mark much of scientific research today. Much less is heard about the genuine cooperation that abounds in the research community, particularly that between men and women from different research centers working toward a common goal.

A telling illustration of close scientific collaboration is the long-standing relationship of laser experts at the Laboratory for Laser Energetics (LLE) of the University of Rochester and at Lawrence Livermore National Laboratory. Their common goal has been to harness the potential of the laser as a future energy source and as a tool for revealing the secrets of matter at extreme temperatures and pressures.

Involved in inertial confinement fusion (ICF) research since the late 1960s, LLE today operates the only fusion research program jointly supported by the federal government, state government, industry, utilities, and a university. The U.S. Department of Energy has designated LLE as the National Laser Users' Facility to enable academic institutions, industrial research establishments, and government laboratories to have access to its facilities.

Showcasing the Omega Laser

LLE's showcase facility is its 60-beam Omega laser, which can deliver more than 40 kilojoules of energy on a target less than 1 millimeter in diameter. (By comparison, the 192-beam National Ignition Facility [NIF], now under construction at Lawrence Livermore, will produce 1.8 megajoules of energy.)

Completed in 1995, Omega is the nation's principal direct-drive laser fusion research facility. With direct drive, laser light strikes a minuscule capsule directly to compress it. In the other approach to inertial fusion—indirect drive—laser light first strikes the inner wall of a metal cylinder called a hohlraum, causing the production of x rays that symmetrically implode a capsule located inside.

Omega is the latest achievement of LLE's laser program, which has paralleled Lawrence Livermore's for nearly four decades. During that time, researchers at each institution have readily adopted the breakthrough technologies developed by the other, often collaborating to improve them or modifying them to suit unique experimental goals. "Such shared technologies translate to a 'national win,'" says LLE director Bob McCrory.

Sharing Improves Technologies and Reduces Cost

When Omega was upgraded from 24 to 60 beams, it married technologies pioneered by both Livermore and LLE. Livermore scientists advised their LLE colleagues about disk amplifier technology they had developed, recalls Howard Powell, Livermore physicist and program leader for Laser Science and Technology. "We told them everything we knew about how to use flashlamps to pump disk amplifiers and how to cool the amplifiers," he says.

Although NIF will use nitrogen gas as a flashlamp coolant, Omega scientists decided to use water. This new technology has paid off—the Omega laser beams have only a 45-minute turnaround time. "The fact that flashlamp cooling works so well for them means we're very confident about using flashlamp cooling techniques for NIF," says Powell.

Livermore laser scientists point to two key developments by their LLE colleagues. The first, achieved in 1980, uses crystals of KDP (potassium dihydrogen phosphate) to efficiently convert a laser's infrared wavelengths to ultraviolet to better couple the laser energy to the target. Early generations of Livermore's neodymium-doped glass lasers—Janus, Cyclops, Argus, and Shiva—produced successively higher peak power and output energy at 1,050-nanometer wavelengths. This wavelength was not short enough to produce effective implosions. Livermore researchers took advantage of the LLE breakthrough in 1985 to convert the laser light on their 10-beam Nova laser to the 351-nanometer wavelength.

McCrory points out that until the Omega upgrade began operation, Nova was the world's most powerful laser. Because of technology advances, Omega was built for roughly one-third the cost of Nova. Further advances make NIF's cost per unit of output energy even lower. NIF has about 60 times the output energy of Omega at roughly 20 times the cost, continuing the trend of advancing technology from Nova to Omega to NIF.

The second major LLE breakthrough was smoothing by spectral dispersion (SSD). This technology shimmers the beam on the target to get rid of speckling and intensity variation, thereby avoiding destructive hot spots. Although it was originally developed for direct-drive experiments, Livermore researchers discovered it was also useful for indirect drive. As a result, SSD was modified and implemented on Nova; it will also be used on NIF.

"The real contest," says McCrory, "is the quality of the laser beam." In that respect, he says, SSD is comparable in importance to Livermore's development of spatial filters in the late 1970s. These filters prevent damage to laser glass by smoothing the shape of and eliminating the high-frequency noise in the beam. At the time, says McCrory, spatial filters were the "salvation" of solid-state lasers.

Omega Stands in for Nova

When Nova was decommissioned in May 1999, Omega became the only facility in the nation doing laser fusion implosion experiments. Although it was designed to do direct-drive experiments, it is working well as a facility for Livermore's indirect-drive experiments.

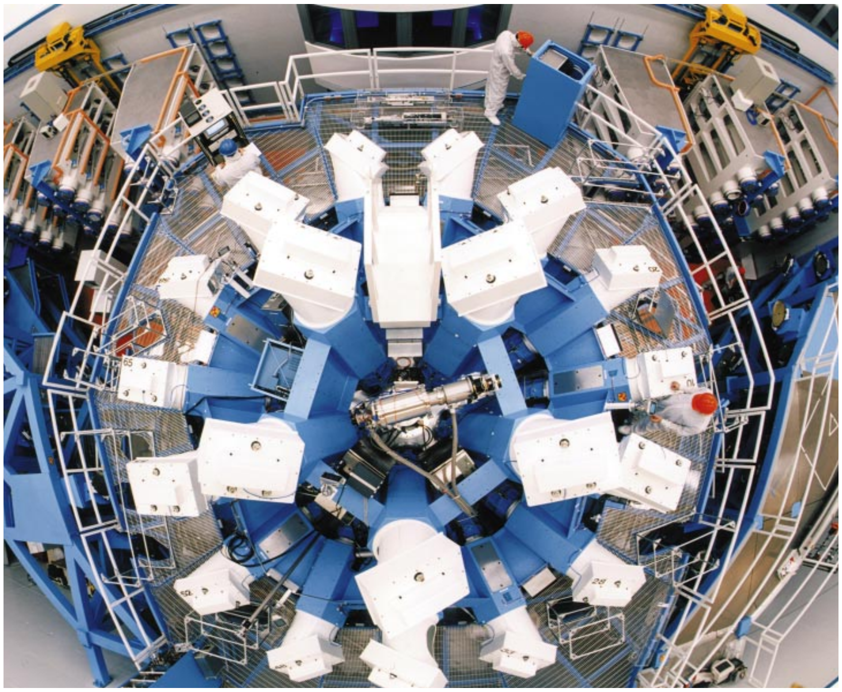
The decision to close Nova and transfer experiments to Omega until NIF begins operation in 2002 was not made lightly. Livermore physicist Ted Perry notes that because Omega was designed as a direct-drive facility, it can use only about 40 of its 60 beams for the indirect-drive targets used on Nova and NIF.

"Omega had to demonstrate that it could do the experiments. It passed all the tests," says Perry, who credits the ingenuity of Livermore and Rochester scientists working together to optimize the facility for indirect drive.

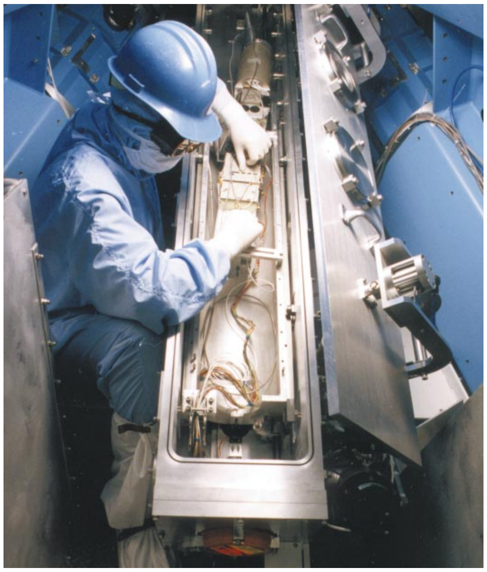
Omega Contributes to Stockpile Stewardship

Most of Livermore's planned shots on Omega for 1999 are earmarked as part of DOE's science-based Stockpile Stewardship Program to ensure that the nation's nuclear weapon stockpile remains safe and reliable. Small Livermore teams travel to Rochester with their laser targets and stay for about a week-long "campaign" of 20 to 30 shots. (Omega averages 10.5 shots per day.)

Most experiments are unclassified, especially fundamental hydrodynamics experiments that can be applied as much to



A view of the Omega target bay from high above the target chamber shows critical components associated with the ultraviolet transport system.



Livermore scientist Ted Perry adjusting a gated x-ray imager on the Omega target chamber. While the National Ignition Facility is being built, teams of Livermore scientists travel to Rochester regularly to do experiments on Omega in support of stockpile stewardship and to advance their understanding of laser target physics.

astrophysics as to understanding nuclear weapons. Diagnostic instrumentation originally built for Nova works well on Omega, thanks to what McCrory calls "shared modularity." In turn, instruments built for Omega can be readily adapted to work on NIF.

Livermore physicists have been impressed with the precision of Omega's 60 beams. "Omega is more precise than Nova because it has more modern technology," says Powell. "Precision is everything in laser fusion."

Livermore physicist Kim Budil points out that Omega's 60 beams give experimenters more flexibility to design experiments than Nova did. What's more, she says, working with the complicated geometry of the beams is good preparation for NIF's 192 beams.

For ICF, it is important that the spherical target stays round as it is squashed by the x rays in the hohlraum. It is relatively easy to detect sausage- and pancake-shaped deviations from spherical implosions, but more complicated deviations from roundness, such as a cross, are harder to measure. A team led by Livermore physicist Nino Landen recently concluded experiments on Omega that demonstrate the detection capability for these subtler deviations, so-called high-order asymmetries, which were difficult, if not impossible, to isolate on Nova. The control of these high-order asymmetries is important to achieving highly spherical implosions and eventually ignition on NIF.

Some Key LLE Accomplishments

1975 to 1976	First direct experiments of compressed fuel density in laser-driven targets.
1975 to 1976	First detailed measurements of ablation and preheat using x-ray line emission.
1975 to 1976	First comprehensive measurements of harmonic and subharmonic emission from spherical targets.
1980	Invention of high-efficiency third-harmonic generation schemes for high-power glass lasers.
1980	First extensive laser–matter interaction experiments with ultraviolet irradiation.
1988	First demonstration of compressions in excess of 100 to 200 times liquid deuterium–tritium density (greater than 20 to 40 grams per cubic centimeter) in thermonuclear fuel using cryogenic targets.
Late 1980s	Pioneering use of SSD (smoothing by spectral dispersion) beam-smoothing technique to produce uniform beam profiles.
1995	Construction of the 60-beam, upgraded Omega laser completed.

In addition to supporting stockpile stewardship experiments by Livermore and Los Alamos personnel, LLE scientists are preparing for direct-drive experiments. McCrory says that LLE is facing the same kinds of technical challenges to make direct-drive work that Nova experimenters faced in the mid-1980s proving indirect drive.

Direct drive is an attractive option to indirect drive because of the potential for higher energy gain, says Charles Verdon, head of the Livermore group that designs laser targets and LLE deputy director from 1994 to 1997. "As Rochester solves its technical issues, such as handling cryogenic targets, the results will help Livermore scientists prepare for NIF," Verdon says. In addition, he says that as a multiuser facility, Omega is serving as a model for how best to operate NIF as a stockpile stewardship facility for all three weapons laboratories.

Omega after NIF

Verdon says that Omega will continue to be an important facility to Livermore even after NIF begins operation. Lawrence Livermore will use Omega to scope out scientific ideas more easily and cheaply. High-power or high-energy experiments, however, will require NIF.

The strong LLE connection to NIF is evident in other areas. LLE optics experts are applying essential multilayer coatings to several NIF optical components, such as the polarizers that form part of the giant laser's optical switches and the deformable mirrors used to control beam quality.

Looking beyond NIF, Livermore and LLE researchers are collaborating on a proposal to develop a DOE "virtual laboratory" to design a diode-pumped solid-state laser for inertial fusion energy. The laser would fire some 10 times per second with 10 percent efficiency. A similar virtual laboratory for a heavy-ion laser facility was formed last year as a collaboration between Livermore and Lawrence Berkeley National Laboratory.

"The ICF program has worked synergistically. There is always pride in ownership, but there haven't been a lot of 'not invented here' roadblocks," says Verdon.

"We compete," adds Powell, "but it's a healthy competition."

—Arnie Heller

Key Words: diode-pumped solid-state laser, direct drive, flashlamp cooling, indirect drive, inertial confinement fusion (ICF), KDP (potassium dihydrogen phosphate) crystals, Laboratory for Laser Energetics (LLE), Lawrence Berkeley National Laboratory, National Ignition Facility (NIF), Nova laser, Omega laser, smoothing by spectral dispersion (SSD), spatial filters.

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Predicting Material Behavior from the Atomic Level Up

MICROSTRUCTURAL features in metals profoundly affect what happens on a larger scale, particularly when systems are pushed to their limits. For example, jet aircraft turbine blades can fail if small concentrations of particular impurities cluster at the boundaries between the individual crystalline grains of the metal. Even in the absence of impurities, the strength and plastic deformation of a metal are controlled by extended crystal defects called dislocations. Such features also affect the performance of nuclear weapon systems, where materials are pushed to extremes of temperatures and pressures.

Modeling macroscopic mechanical properties such as strength and failure at different length scales—that is, multiscale modeling—is of major interest at Lawrence Livermore because of its relevance to the Department of Energy's Stockpile Stewardship Program. With the cessation of underground nuclear testing, weapons scientists must be able to predict with confidence the properties of materials in stockpiled warheads and their effect on weapons performance.

This need to predict performance has put a high premium on understanding materials behavior. In this respect, the mechanical properties of nuclear weapon materials are uniquely complex. Unlike thermodynamic properties, such as the equation of state, which are fully determined at the atomic length scale, mechanical properties are inherently multiscale, depending on phenomena at all length scales. Thus, multiscale modeling is a huge scientific challenge as well as a critical necessity for successful stockpile stewardship. To meet these demands, Livermore's multiscale-modeling effort involves some 25 researchers from a variety of disciplines (theoretical and weapons physics, engineering, and chemistry and materials science) as well as many outside collaborators, including the Massachusetts Institute of Technology, Stanford University, the University of California at Los Angeles, the University of Illinois, Brown University, Yale University, Carnegie–Mellon University, and IBM.

Making Connections among Scales

In the multiscale program, scientists are creating and validating computer models to predict and explain the mechanical properties of metals at dimensions ranging from a fraction of a nanometer to meters. The focus is on three major length scales—the atomic scale (nanometers), the microscale (micrometers), and the mesoscale (millimeters and above) (Figure 1). What sets this effort apart from previous ones is that fundamental physical and mathematical principles are rigorously applied to the modeling at each scale, and data are then passed to the next scale up. In the past, such efforts were hampered by the lack of computational power needed to simultaneously model the individual and collective behavior of a large number of atoms and defects. Now, by combining a multiscale-modeling strategy with spectacular advances in computational technology, scientists are shedding light on the fundamental mechanisms that determine how materials deform and fail.

John Moriarty, a leading physicist in Livermore's multiscale-modeling effort, notes, "In the days of underground weapons testing, hydrodynamic computer codes relied on purely phenomenological models of mechanical properties based upon limited experimental data obtained at or near ambient conditions. In the multiscale-modeling program, we are developing a predictive capability based on first principles. That is, the predictions we make at the everyday macroscopic level will be based on fundamental quantities and rules derived from the atomic scale and microscale."

The program is currently focused on the prototype problem of strength and plastic deformation in body-centered-cubic (bcc) metals, such as molybdenum and tantalum (Figure 2). These metals are of special interest because of their physical and structural similarity to stockpile materials. Tantalum, in particular, is predicted to remain a bcc metal to extremely high pressures. In addition, notes Moriarty, the thermodynamic and mechanical properties of metals such as tantalum are of long-standing interest to both the high-pressure and materials physics communities.

Over the years, the materials scientists have accumulated substantial data on the yield strength and other mechanical properties of bcc metals at or near ambient pressure, and more detailed and accurate data are being obtained as part of the multiscale program. Theoretical corroboration has been lacking, however, as has information on tantalum's mechanical properties at high pressures. Rigorous

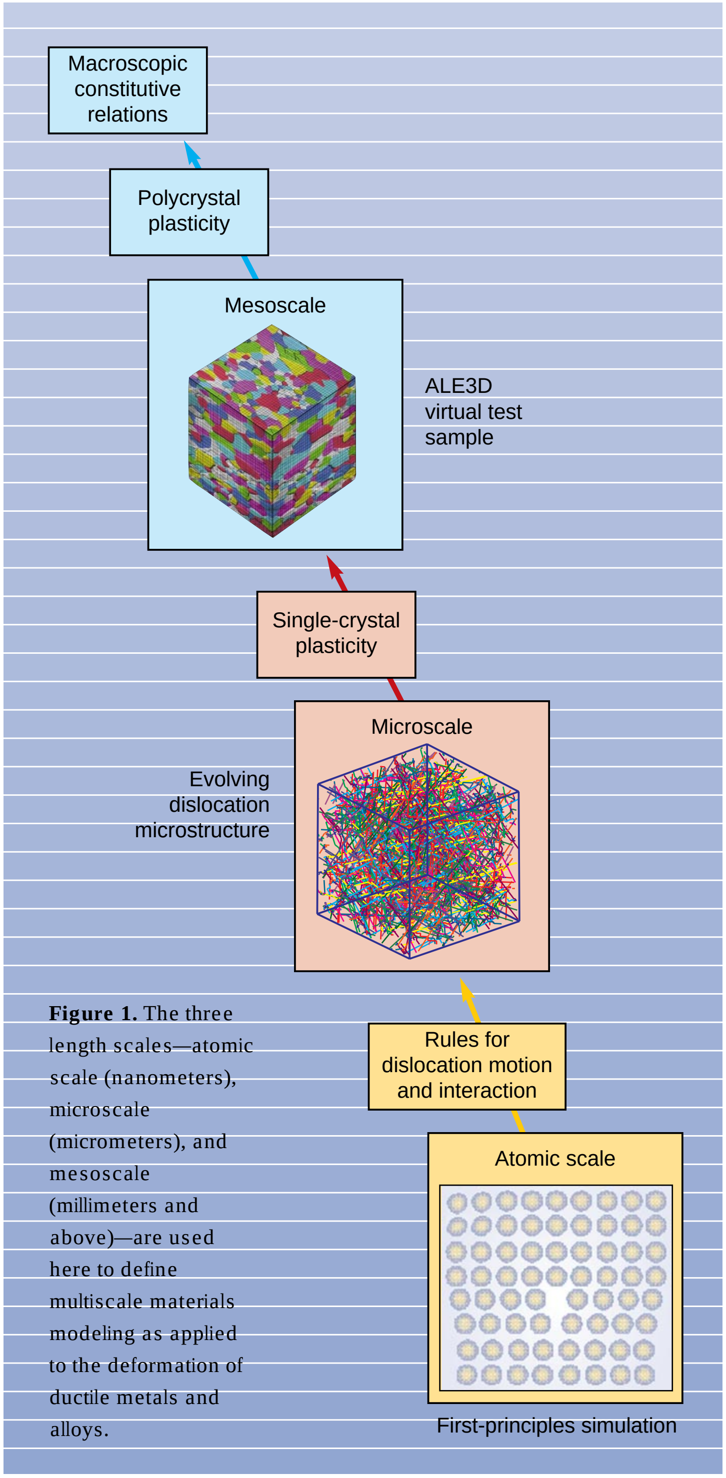

Figure 1. The three length scales—atomic scale (nanometers), microscale (micrometers), and mesoscale (millimeters and above)—are used here to define multiscale materials modeling as applied to the deformation of ductile metals and alloys.

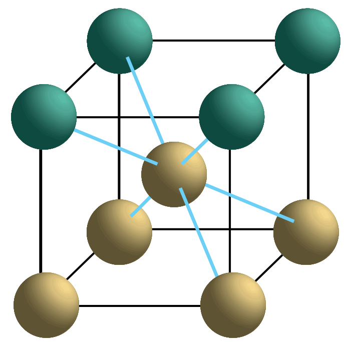

Figure 2. A body-centered-cubic (bcc) crystal. Tantalum and molybdenum are examples of metals with a bcc crystal structure.

mathematical answers are difficult to come by because mechanical properties depend on phenomena at all length scales. The advent of the Department of Energy's Accelerated Strategic Computing Initiative means that the computational power is now available to bridge the different length scales and accurately model the mechanical properties of tantalum and other metals from first principles.

Climbing the Multiscale-Modeling Ladder

To define the plastic deformation problem in detail, multiscale modelers use a top-down strategy to pose questions and a bottom-up strategy to obtain solutions. Modeling at each length scale helps pose critical questions to be addressed at the next lower scale. To achieve the corresponding solution, appropriate simulations at the atomic scale, for example, provide input at the microscale.

For tantalum, Moriarty and others start with its fundamental atomic properties, using rigorous quantum-mechanical principles and first-principles calculations to develop accurate interatomic force laws that can be applied to atomistic simulations involving many thousands of atoms. From these simulations, they derive the properties of individual dislocations in a perfect crystal and then, with new microscale simulation techniques, look at the behavior of large collections of interacting dislocations at the microscale in a grain-sized crystal. They model the grain interactions in detail with finite-element simulation codes, and from those simulations, they finally construct appropriate models of properties such as yield strength in a macroscopic chunk of tantalum. At each length scale, the models are experimentally tested and validated with available data. Once validated, the models can be used to predict behavior in regimes not achievable in the laboratory.

The challenge at the atomistic level is to learn how individual dislocations move and interact in the presence of an applied stress. Dislocations—which appear as extra or displaced planes of atoms inserted into the regular latticelike structure of a metal crystal—allow otherwise crystalline material to deform plastically without brittle fracture or failure. Figure 3 shows examples of edge and screw dislocations. Edge dislocations resemble an extra sheet of paper slipped part way into a stack of sheets. In a screw dislocation, the atomic planes are twisted like the steps of a spiral staircase.

The energy of a dislocation is stored largely as strain in the surrounding lattice. The important property of a dislocation is its ability to move easily through the lattice, allowing slip to propagate rapidly. (Slip, or the movement of one atomic plane over another, is the primary way that plastic deformation occurs in a solid.) In bcc metals, screw dislocations limit plastic flow because they are much less mobile than edge dislocations, especially at low temperature or under high strain-rate deformation conditions.

Progress So Far

To date, the team has calculated a wide range of deformation and defect properties for tantalum, validated those calculations, and carried them up to extremely high pressures for many of those properties, including bcc elastic constants. At ambient pressure, the elastic constants agree with measured values. Experiments are under way to measure these quantities at high pressure. Atomistic simulations have been used to predict the atomic structure of selected grain boundaries in niobium, molybdenum, and tantalum. The predicted structures in niobium and molybdenum were confirmed by high-resolution electron microscopy (HREM) experiments, and additional experiments on tantalum are in progress.

The team has also used atomistic simulations to study fundamental properties of screw and edge dislocations in molybdenum and tantalum at ambient pressure. The simulations predicted atomic core structures with unique threefold spreading for the screw dislocations; for molybdenum, this spreading was recently confirmed by HREM experiments in Germany. The minimum, or Peierls, stress required to move these screw dislocations has also been studied as a function of the orientation of the applied stress. This minimum stress can be further reduced by forming local excitations called kinks along the dislocation line, and a study of kink energetics leading to dislocation mobility is in progress.

Bridging Length-Scale Worlds

Microscale modeling bridges the atomic and mesoscale worlds. At the microscale, researchers are developing entirely new three-dimensional, dislocation-dynamics (DD) simulation techniques to model single 15-micrometer-long crystals. In these simulations, dislocation structures are resolved, but individual atoms are not, and the basic building blocks are small segments of individual dislocations. In DD simulations, dislocations move and interact according to linear elasticity laws as well as rules established by atomistic simulations and fine-grained DD simulations of small numbers of dislocations.

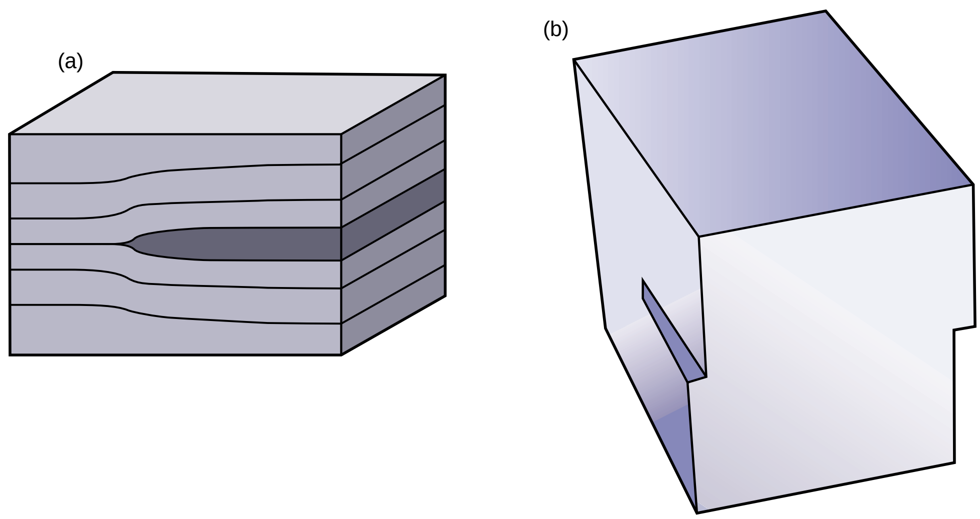

Figure 3. Representation of (a) an edge dislocation and (b) a screw dislocation.

(a) (b)

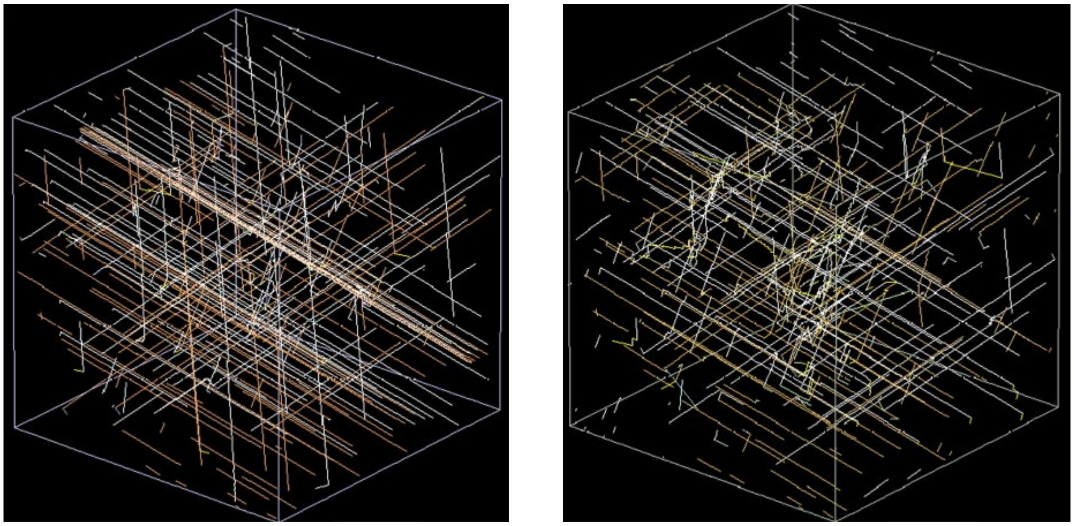

Figure 4. Three-dimensional simulations of dislocation structures in body-centered-cubic tantalum at (a) 197 kelvins and (b) 300 kelvins. The long, straight segments are screw dislocations, while the majority of short segments are edge dislocations.

Developing these rules rigorously is one of the most difficult aspects of the multiscale program. A complementary experimental program is examining dislocation microstructures with transmission electron microscopy and providing stress–strain data on well-characterized, high-purity samples.

The DD simulations provide insights and detailed information about the collective behavior of large numbers of interacting dislocations. They also simulate the evolution of a complex dislocation microstructure under an applied stress (Figure 4). Adds Moriarty, "Dislocations and their distribution are an essential part of plastic deformation. But never before has there been such a powerful tool to model this phenomenon." In the multiscale strategy, the goal at the microscale is to provide a full quantitative description of single-crystal plasticity, including the yield stress and stress–strain relationships. With currently available phenomenological input, the DD simulations have provided accurate results for the single-crystal yield stress in tantalum, including its temperature dependence.

The derived laws of single-crystal plasticity will ultimately be used in mesoscale-modeling simulations to predict the deformation of millimeter-sized tantalum polycrystals, that is, multiple single crystals with different orientations packed together into a single specimen. In mesoscale modeling, the individual crystals and their boundaries are resolved, but microstructures and individual dislocations are not. At this scale, scientists are using finite-element simulation codes such as NIKE3D and ALE3D to examining how a system of randomly arranged, computer-generated single crystals—a virtual test sample—deforms in response to an applied stress. The mesoscale-modeling results will finally be used to derive constitutive relations that describe macroscopic plasticity.

The multiscale-modeling program expects to complete its task in about eight more years, linking quantum-based atomistic models all the way up to finite-element-based mesoscopic simulations. When complete, the models will help stockpile stewardship scientists confidently predict the performance of stored weapons and changes that might occur in the stockpile, as well as provide basic information about material behavior of interest to the nation's industrial products manufacturers.

—Ann Parker

Key Words: atomic scale modeling, body-centered-cubic (bcc) crystal structure, dislocation dynamics (DD), edge dislocation, mesoscale modeling, microscale modeling, multiscale modeling, polycrystals, screw dislocation, stockpile stewardship, transmission electron microscopy.

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